

Generalized Version of the Creation and Annihilation Operators for the Schrödinger Equation

Santos, L. C. N^{a,*}, C.C. Barros Jr^{a,*}

^a*Departamento de Física - CFM - Universidade Federal de Santa Catarina, Florianópolis - SC - CP. 476 - CEP 88.040 - 900 - Brazil.*

Abstract

A generalized version of the creation and annihilation operators is constructed and the factorization of the Schrödinger equation is investigated. It is shown that the generalized version of factorization operators yield a factorization for the twelve different separable coordinates for the Schrödinger equation.

Keywords: , factorization method, Schrödinger equation, operators

1. Introduction

The factorization method, introduced by Schrödinger [1] and Dirac [2] and later developed by Infeld and Hull [3], is one of the methods for solving quantum mechanical problems. The idea is to consider a pair of first-order differential
 5 equations which are equivalent to a given second-order differential equation. The complete set of normalized eigenfunctions can be obtained by the successive application of the ladder operators on the eigenfunctions, which are the exact solutions of the first order differential equation.

From the 1970s to the early 1980, it was a common opinion that the method
 10 was completely explored. However, Mielnik made an additional contribution to the traditional factorization method in 1984 [4]. In that work, he did not consider the particular, but the general solution to the Riccati type equation

*Corresponding author

Email addresses: `luis.santos@ufsc.br` (Santos, L. C. N), `barros.celso@ufsc.br` (C.C. Barros Jr)

connected with the Infeld-Hull approach. Mielnik factorization is a powerful tool in the derivation of new Hamiltonians whose corresponding eigenproblem
15 is analytically solvable. On the other hand, the connection between the Infeld method and supersymmetric quantum mechanics (SUSY QM) has been explored by many authors [5, 6, 7, 8]. For example, Witten noticed the possibility of arranging the second-order differential equations into isospectral pairs, the so-called supersymmetric partners.

20 In many works, the factorization method has been used as a tool to formulate algebraic approaches to many non-relativistic quantum problems, the idea is build sets of one variable radial operators which are realizations for $su(1, 1)$ Lie algebra [9, 10]. The separable coordinate systems for the Schrödinger equation are confocal quadric surfaces [11], and the potential is a function of the
25 coordinates [12].

In this paper, the possibility of factorization of the separated equations is investigated, and it is shown that a generalized version of the creation and annihilation operators can be constructed. Indeed, these operators yield a factorization for the twelve different separable coordinates for the Schrödinger equation. In the Infeld method, the original form of the second-order differential equation

$$\frac{d}{d\theta} \left(p \frac{d\psi}{d\theta} \right) + q(\theta) \psi + \lambda \rho(\theta) \psi = 0, \quad (1)$$

is transformed in the form

$$\frac{d^2 y}{dx^2} + r(x, m) y + \lambda y = 0, \quad (2)$$

where $m = 1, 2, 3, \dots$ and p, ρ are positive functions. The transformation connecting these equations is

$$y = (p\rho)^{1/2} \psi, \quad dx = (\rho/p)^{1/2} d\theta. \quad (3)$$

In this work, we propose to apply a factorization method for the original form of the separated Schrödinger equation. In this way, our approach yield factorization operators for the twelve different separable coordinate systems. An

interesting feature of this work is that the original Hilbert space of theory is
 30 sustained.

So, this paper will show the following contents: In section II, we enumerate
 the coordinates systems which will allow separation of the Schrödinger equation.
 In section III, a generalized version of the creation and annihilation operators is
 proposed. In section IV and V, we apply the method to the radial second-order
 35 Schrödinger equation.

2. Separable coordinate systems for the wave equation

In this section, we study the separable coordinate systems for the Schrödinger
 equation, for more details and information see [13]. We consider the standard
 differential equation for the scalar field

$$\nabla^2\psi + k_1^2\psi = 0, \quad (4)$$

where ∇^2 is the Laplace operator. When k_1 is a function of the coordinates, we
 obtain the Schrödinger equation. The rectangular coordinates x, y, z and the
 curvilinear coordinates ξ_1, ξ_2, ξ_3 are related by the scale factors

$$h_n = \sqrt{\left(\frac{\partial x}{\partial \xi_n}\right)^2 + \left(\frac{\partial y}{\partial \xi_n}\right)^2 + \left(\frac{\partial z}{\partial \xi_n}\right)^2}, \quad (5)$$

where $n = 1, 2, 3$. The Laplacian can be expressed in its generalized form

$$\nabla^2\psi = \sum_n \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial \xi_n} \left[\frac{h_1 h_2 h_3}{h_n^2} \frac{\partial \psi}{\partial \xi_n} \right], \quad (6)$$

thus we can rewrite the equation (4) into

$$\sum_n \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial \xi_n} \left[\frac{h_1 h_2 h_3}{h_n^2} \frac{\partial \psi}{\partial \xi_n} \right] + k_1^2\psi = 0. \quad (7)$$

In order to obtain the separated equations, we introduce the Stäckel deter-

minant

$$\begin{aligned}
S = |\Phi_{mn}| &= \begin{vmatrix} \Phi_{11} & \Phi_{12} & \Phi_{13} \\ \Phi_{21} & \Phi_{22} & \Phi_{23} \\ \Phi_{31} & \Phi_{32} & \Phi_{33} \end{vmatrix} \\
&= \Phi_{11}\Phi_{22}\Phi_{33} + \Phi_{12}\Phi_{23}\Phi_{31} + \Phi_{13}\Phi_{21}\Phi_{32} \\
&\quad - \Phi_{13}\Phi_{22}\Phi_{31} - \Phi_{11}\Phi_{23}\Phi_{32} - \Phi_{12}\Phi_{21}\Phi_{33},
\end{aligned} \tag{8}$$

where Φ_{mn} are functions of ξ_n alone.

If the separated equations for the three-dimensional case are

$$\frac{1}{f_m(\xi_m)} \frac{d}{d\xi_m} \left[f_m(\xi_m) \frac{dX_m}{d\xi_m} \right] + \sum_n \Phi_{mn}(\xi_m) k_n^2 X_m = 0, \tag{9}$$

we can relate the equations (7) and (9) by the Robertson condition [13]

$$\frac{h_1 h_2 h_3}{S} = f_1(\xi_1) f_2(\xi_1) f_3(\xi_1),$$

which limits the kinds of coordinates systems which will allow separation. The

equation (9) is supposed to be a separated equation, therefore the functions f_n ,

40 Φ_{n1} , Φ_{n2} , and Φ_{n3} must all be functions of ξ_n alone.

3. Creation and annihilation operators

In this section, we propose a generalized version of the creation and annihilation operators. For the Schrödinger equation the constant k_1 must have the form $k_1^2 = \varepsilon - \sum_n^3 v_n(\xi_n)$ [13], where $v_n(\xi_n) = \frac{2m}{\hbar^2} V_n(\xi_n)$, substituting it into the equation (9) gives

$$\begin{aligned}
&\frac{1}{f_m(\xi_m)} \frac{d}{d\xi_m} \left[f_m(\xi_m) \frac{dX_m}{d\xi_m} \right] + \\
&\Phi_{m1}(\xi_m) \left[\varepsilon - \sum_n^3 v_n(\xi_n) \right] X_m + \\
&\Phi_{m2}(\xi_m) k_2^2 X_m + \Phi_{m3}(\xi_m) k_3^2 X_m = 0.
\end{aligned} \tag{10}$$

Introducing $k'_1 = \varepsilon$, $k_2 = k'_2$, $k_2 = k'_2$ into (10) we obtain

$$\begin{aligned} & \frac{1}{f_m(\xi_m)} \frac{d}{d\xi_m} \left[f_m(\xi_m) \frac{dX_m}{d\xi_m} \right] \\ & + \sum_{m \neq n}^3 k_m'^2 \Phi_{nm}(\xi_m) X_n - v_n X_n \\ & = k_n'^2 \Phi_{nn} X_n. \end{aligned} \quad (11)$$

These are the separated equations for the three-dimensional space. Now we propose to apply a factorization method for the separated Schrödinger equation (11). The idea is to define two ladder operators

$$A = \frac{d}{d\xi_m} + \frac{1}{2f_m} \frac{df_m}{d\xi_m} - R(\xi_m), \quad (12)$$

$$A^+ = \frac{d}{d\xi_m} + \frac{1}{2f_m} \frac{df_m}{d\xi_m} + R(\xi_m), \quad (13)$$

and to show that these operators yield a factorization of the equation (11).

Indeed, if we multiply A by A^+ , we find

$$\begin{aligned} AA^+ &= \frac{1}{f_m} \frac{d}{d\xi_m} \left(f_m \frac{dX_m}{d\xi_m} \right) - \frac{1}{4f_m^2} \left(\frac{df_m}{d\xi_m} \right)^2 \\ &+ \frac{1}{2f_m} \frac{d^2 f_m}{d\xi_m^2} + R' - R^2, \end{aligned} \quad (14)$$

and comparing with equation (11) we find a Riccati type equation

$$R' - R^2 = \epsilon + \Gamma(\xi_n), \quad (15)$$

where ϵ is a constant and

$$\Gamma(\xi_n) = \frac{1}{4f_m^2} \left(\frac{df_m}{d\xi_m} \right)^2 - \frac{1}{2f_m} \frac{d^2 f_m}{d\xi_m^2} + \sum_{m \neq n}^3 k_m'^2 \Phi_{nm} - v_n. \quad (16)$$

The occurrence of the Riccati equation in the factorization of second-order differential equations is a typical phenomenon. Specifically, the factorization operators convert the equation (11) into product of A and A^+ with a extra condition, a Riccati type equation. The explicit solution of this type of equation, in ge-neral, is not Known [14]. In the following, we will obtain two particular solutions of the Riccati equation (15) in a spherical coordinate system for the Coulomb and isotropic oscillator potentials.

4. Application to hydrogen atom

We want to show how to solve the radial Schrödinger equation with Coulomb potential. We apply the method to the radial second-order differential equation, in this case, the spherical coordinates are denoted by $\xi_1 = r$, $\xi_2 = \theta$, $\xi_3 = \phi$ and the f_n functions are $f_1 = r^2$, $f_2 = 1 - \cos^2 \theta$, $f_3 = \sqrt{1 - \cos^2 \phi}$. Therefore the s matrix is given by

$$S = \begin{pmatrix} 1 & \frac{1}{r^2} & 0 \\ 0 & \frac{1}{\cos^2 \theta - 1} & \frac{1}{(\cos^2 \theta - 1)^2} \\ 0 & 0 & \frac{1}{\cos^2 \phi - 1} \end{pmatrix}. \quad (17)$$

The separation constants are then required to be of the form

$$k_1^2 = \varepsilon, \quad k_2^2 = -l(l+1), \quad k_3^2 = m.$$

So the radial Schrödinger equation with potential $v_n = -K/r$ is

$$\frac{d^2 X_1}{dr^2} + \frac{2}{r} \frac{dX_1}{dr} - \frac{l(l+1)}{r^2} + \frac{K}{r} = -\varepsilon X_1, \quad (18)$$

and the Ricatti equation is

$$R' - R^2 = \varepsilon - \frac{l(l+1)}{r^2} + \frac{K}{r}, \quad (19)$$

the particular solution for this equation is given by

$$R = \frac{l}{r} - \frac{K}{2l},$$

where $\varepsilon = -\frac{K^2}{4l^2}$. The creation and annihilation operators in (12) and (13) can be written in the form

$$\begin{aligned} A_l^+ &= \frac{d}{dr} + \frac{1}{r} + \frac{l}{r} - \frac{K}{2l}, \\ A_l &= \frac{d}{dr} + \frac{1}{r} - \frac{l}{r} + \frac{K}{2l}. \end{aligned}$$

The commutator of A_l and A_l^+ is r dependent

$$[A_l^+, A_l] = A_l^+ A_l - A_l A_l^+ = \frac{2l}{r^2}. \quad (20)$$

Indeed, the A_l and A_l^+ are creation and annihilation operators. We can prove this directly, the first step is to consider the product between the operators $A_l^+ A_l$ and the radial wave function $X_{n,l-1}$, i.e,

$$\begin{aligned} A_l^+ A_l X_{n,l-1} &= \left(H_{l-1} - \frac{K^2}{4l^2} \right) X_{n,l-1} \\ &= \left(\varepsilon_{n,l-1} - \frac{K^2}{4l^2} \right) X_{n,l-1}, \end{aligned} \quad (21)$$

in a similar way

$$\begin{aligned} A_l A_l^+ X_{n,l} &= \left(H_l - \frac{K^2}{4l^2} \right) X_{n,l} \\ &= \left(\varepsilon_{n,l} - \frac{K^2}{4l^2} \right) X_{n,l}. \end{aligned} \quad (22)$$

A direct calculation shows that these operators satisfy

$$[H_l, A_l] = \frac{2l}{r^2} A_l \quad (23)$$

and

$$[H_{l-1}, A_l^+] = -\frac{2l}{r^2} A_l^+, \quad (24)$$

so the action of the A_l and H_l on the states $X_{n,l}$ is

$$\begin{aligned} H_l A_l X_{n,l} &= A_l \left(\frac{2l}{r^2} + H_l \right) X_{n,l} \\ &= \varepsilon_{n,l-1} A_l X_{n,l}, \end{aligned} \quad (25)$$

this result imply

$$X_{n,l-1} \propto A_l X_{n,l}$$

or

$$X_{n,l-1} = c A_l X_{n,l}, \quad (26)$$

where c is a constant. Equivalently

$$X_{n,l} = c A_l^+ X_{n,l-1}. \quad (27)$$

These results imply that the action of the operators A_l and A_l^+ on the states $X_{n,l}$ and $X_{n,l-1}$ is to change the quantum number l . In order to determinate c , we apply A_l to the left-hand side of eq. (27)

$$A_l X_{n,l} = c A_l A_l^+ X_{n,l-1} \quad (28)$$

Therefore, using equation (26) we find

$$c = \frac{1}{\sqrt{(\varepsilon_{n,l} - \frac{K^2}{4l^2})}}. \quad (29)$$

50 5. Radial harmonic oscillator

Solutions of equation (11) are limited to a small set of potentials and the radial harmonic oscillator is one of the few quantum systems where an exact and analytical solution is known. The time-independent Schrödinger radial equation for the isotropic oscillator $v_n = kr^2$ reads

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} - kr^2 \right] X_1 = -\varepsilon X_1, \quad (30)$$

for this case, the Riccati equation is

$$R' - R^2 = \epsilon - \frac{l(l+1)}{r^2} - kr^2 \quad (31)$$

the particular solution of equation (31) is given by

$$R = \frac{l}{r} - \sqrt{kr}, \quad \epsilon = \sqrt{k}(2l-1). \quad (32)$$

This solution R leads to factorizing operators

$$A_l = \frac{d}{dr} + \frac{1}{r} - \frac{l}{r} + \sqrt{kr}, \quad (33)$$

and

$$A_l^+ = \frac{d}{dr} + \frac{1}{r} + \frac{l}{r} - \sqrt{kr}. \quad (34)$$

Hence, we get the following commutation rules

$$[A_l^+, A_l] = \frac{2l}{r} + 2\sqrt{k}$$

and

$$\begin{aligned} [H_l, A_l] &= A_l [A_l^+, A_l] \\ &= A_l \left(\frac{2l}{r} + 2\sqrt{k} \right), \end{aligned} \quad (35)$$

$$\begin{aligned}
[H_{l-1}, A_l^+] &= A_l^+ [A_l, A_l^+] \\
&= -A_l^+ \left(\frac{2l}{r} + 2\sqrt{k} \right),
\end{aligned} \tag{36}$$

thus, the action of the A_l and H_l on the states $X_{n,l}$ is

$$H_l A_l X_{n,l} = \varepsilon_{n,l-1} A_l X_{n,l}. \tag{37}$$

Equivalently, the action of the A_l^+ and H_{l-1} on the states $X_{n,l-1}$ leads to

$$H_{l-1} A_l^+ X_{n,l-1} = \varepsilon_{n,l} A_l^+ X_{n,l-1}, \tag{38}$$

thus, A_l^+ and A_l are the raising and lowering operators for the isotropic oscillator. It follows that

$$X_{nl-1} = c A_l X_{nl}, \quad X_{nl} = c A_l^+ X_{nl-1}, \tag{39}$$

where

$$c = \frac{1}{\sqrt{\varepsilon_{nl} + \sqrt{k}(2l-1)}}.$$

6. Summary and conclusions

In this paper, we have determined the separable coordinate systems for the Schrödinger equation. From these results, factorization operators for the twelve different separable coordinates have been provided. We have determined the Schrödinger equation in the presence of a Coulomb potential and a radial harmonic oscillator potential. We have shown that, a new set of generalized creation and annihilation operators has been introduced. By using the apparatus developed in this work, we believe that other potentials in different coordinate systems can be solved. We conclude by mentioning that links between supersymmetric quantum mechanics and non-linear ordinary differential equations as the Riccati equation (15) can be established [15].

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